2-Anilino-3,6-dimethyl pyrazine

Inchi: InChI=1S/C12H13N3/c1-9-8-13-10(2)12(14-9)15-11-6-4-3-5-7-11/h3-8H,1-2H3,(H,14,15)
InchiKey: POVOGNYQAMJQOM-UHFFFAOYSA-N
Formula: C12H13N3
SMILES: Cc1cnc(C)c(=Nc2ccccc2)[nH]1
Mol. weight [g/mol]: 199.25
CAS: 116659-96-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Crippen Method
logp	1.777		Crippen Method
mcvol	162.360	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659962&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume